

This is a repository copy of *Erratum: Improved real-space genetic algorithm for crystal structure and polymorph prediction [Phys. Rev. B 77, 134117 (2008)]*.

White Rose Research Online URL for this paper:

<https://eprints.whiterose.ac.uk/108601/>

Version: Accepted Version

Article:

Abraham, N. L.. and Probert, Matthew Ian James orcid.org/0000-0002-1130-9316 (2016) Erratum: Improved real-space genetic algorithm for crystal structure and polymorph prediction [Phys. Rev. B 77, 134117 (2008)]. Physical Review B. 059904. p. 1. ISSN 2469-9969

<https://doi.org/10.1103/PhysRevB.94.059904>

Reuse

Items deposited in White Rose Research Online are protected by copyright, with all rights reserved unless indicated otherwise. They may be downloaded and/or printed for private study, or other acts as permitted by national copyright laws. The publisher or other rights holders may allow further reproduction and re-use of the full text version. This is indicated by the licence information on the White Rose Research Online record for the item.

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.

**Erratum: Improved real-space genetic algorithm for crystal
structure and polymorph prediction [Phys. Rev. B 77, 134117
(2008)]**

E. J. Higgins and M. I. J. Probert

Department of Physics, University of York, York, YO10 5DD, UK

(Dated: July 20, 2016)

In the original paper, there was an error in the derivation of the spherically averaged scattering intensity, presented in Eq. (5) in the original paper. This equation should have read:

$$\Lambda(k_r) = \sum_{n=1}^N \rho'(n)^2 + 2 \sum_{n=1}^N \sum_{m>n}^N \rho'(n)\rho'(m)j_0(k_r|\mathbf{r}_n - \mathbf{r}_m|) \quad (1)$$

where $j_0(r)$ is the spherical Bessel function of the 1st kind.

The consequence of using the incorrect equation is that the R-factor behaved significantly differently for calculations with varying volumes, and also had an imbalance between the two terms which skewed the results.

Figure 1 shows the R-factor when comparing a reference 8-atom silicon unit cell to a perturbed copy of that cell. In the replica, the atomic positions, and optionally cell vectors, have been randomly perturbed up to some amount Δx . The original equation can give significantly different results for similar structures in fixed and variable cell calculations.

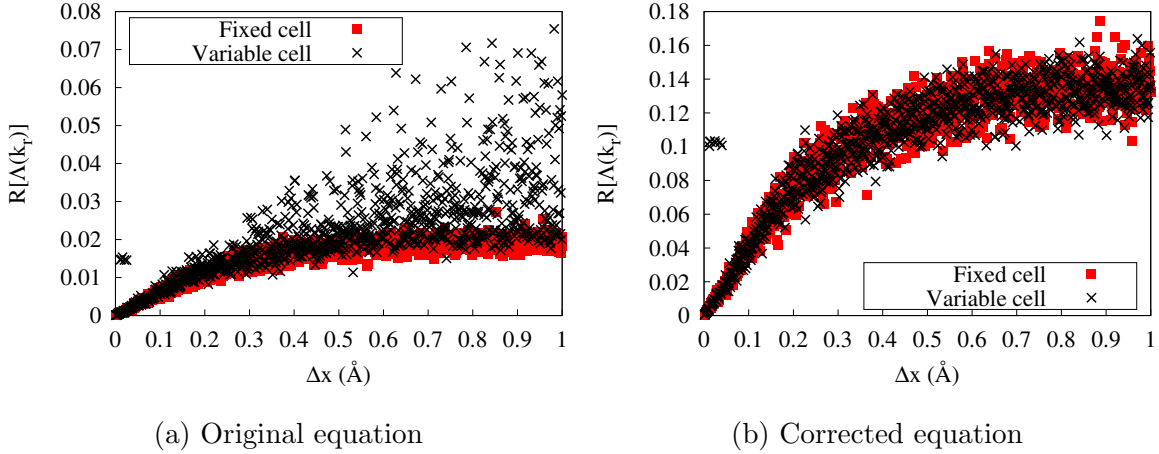


FIG. 1: R-factor vs. perturbation size for an 8-atom unit cell, using (a) the original and (b) the corrected scattering intensities.

As a result of this error, structures of different volumes will give incorrect R-factors. This may have slowed the convergence of the GA calculations presented in the original paper.